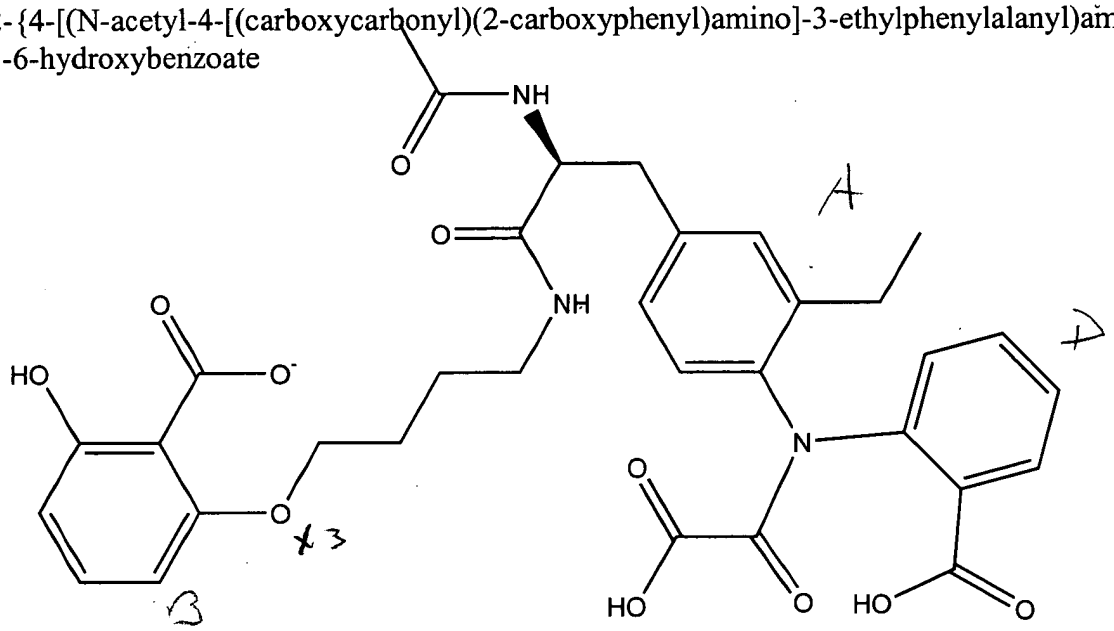
2-{4-[(N-acetyl-4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenylalanyl)amino]butoxy}-6-hydroxybenzoate



2-{4-[(N-acetyl-4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenylalanyl)amino]butoxy}-6-hydroxybenzoate

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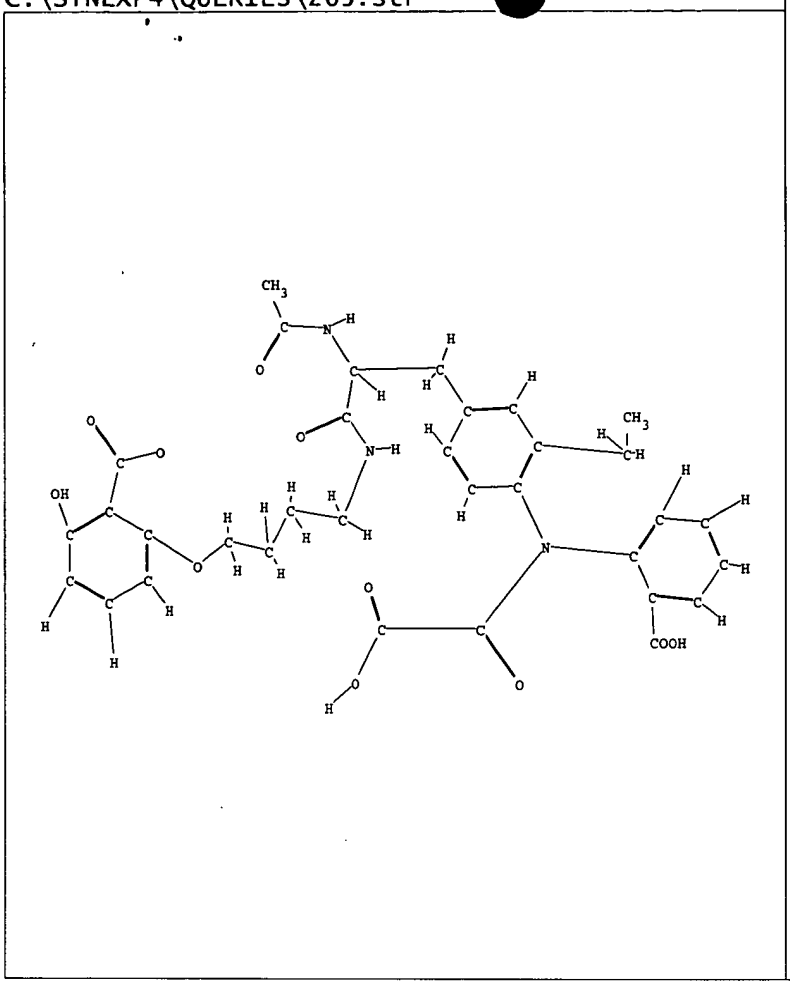

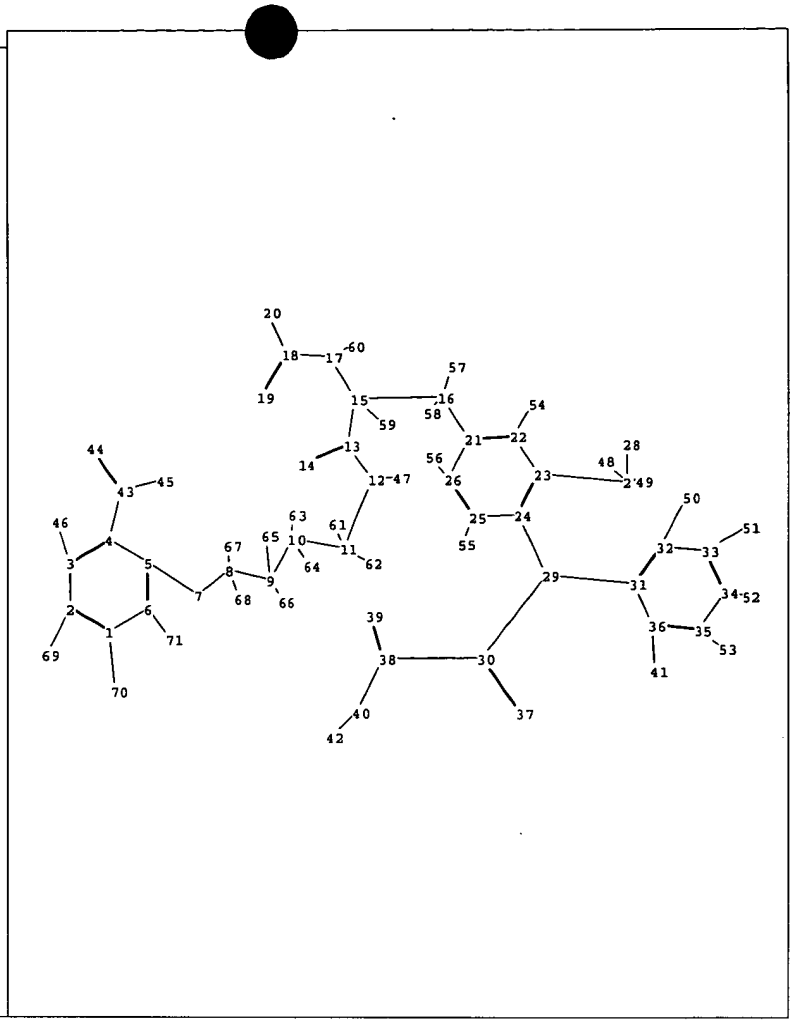

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chain nodes :
    7  8  9  10  11  12  13  14  15  16  17  18  19  20  27  28  29  30  37  38  39  40  41  42
    43  44  45  46  47  48  49  50  51  52  53  54  55  56  57  58  59  60  61  62  63  64  65
    66  67  68  69  70  71
ring nodes :
    1  2  3  4  5  6  21  22  23  24  25  26  31  32  33  34  35  36
chain bonds :
    1-70  2-69  3-46  4-43  5-7  6-71  7-8  8-9  8-67  8-68  9-10  9-65  9-66  10-11  10-63
    10-64  11-12  11-61  11-62  12-13  12-47  13-14  13-15  15-16  15-17  15-59  16-21  16-57
    16-58  17-18  17-60  18-19  18-20  22-54  23-27  24-29  25-55  26-56  27-28  27-48  27-49
    29-30  29-31  30-37  30-38  32-50  33-51  34-52  35-53  36-41  38-39  38-40  40-42  43-44
    43-45
ring bonds :
    1-2  1-6  2-3  3-4  4-5  5-6  21-22  21-26  22-23  23-24  24-25  25-26  31-32  31-36  32-33
    33-34  34-35  35-36
exact/norm bonds :
    3-46  5-7  7-8  11-12  12-13  13-14  15-17  17-18  18-19  24-29  29-30  29-31  30-37  43-44
    43-45
exact bonds :
    1-70  2-69  4-43  6-71  8-9  8-67  8-68  9-10  9-65  9-66  10-11  10-63  10-64  11-61
    11-62  12-47  13-15  15-16  15-59  16-21  16-57  16-58  17-60  18-20  22-54  23-27  25-55
    26-56  27-28  27-48  27-49  30-38  32-50  33-51  34-52  35-53  36-41  40-42
normalized bonds :
    1-2  1-6  2-3  3-4  4-5  5-6  21-22  21-26  22-23  23-24  24-25  25-26  31-32  31-36  32-33
    33-34  34-35  35-36  38-39  38-40


Match level :
    1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:CLASS
    11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:CLASS  19:CLASS
    20:CLASS  21:Atom  22:Atom  23:Atom  24:Atom  25:Atom  26:Atom  27:CLASS  28:CLASS
    29:CLASS  30:CLASS  31:Atom  32:Atom  33:Atom  34:Atom  35:Atom  36:Atom  37:CLASS
    38:CLASS  39:CLASS  40:CLASS  41:CLASS  42:CLASS  43:CLASS  44:CLASS  45:CLASS  46:CLASS
    47:CLASS  48:CLASS  49:CLASS  50:CLASS  51:CLASS  52:CLASS  53:CLASS  54:CLASS  55:CLASS
    56:CLASS
```

57:CLASS 58:CLASS 59:CLASS 60:CLASS 61:CLASS [redacted]CLASS 63:CLASS 64:CLASS
65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS 71:CLASS

L6 2 SEA SSS FUL L5

L7 2 L6

=> d l7 1-2 ibib abs hitstr

L7 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:869580 CAPLUS
DOCUMENT NUMBER: 137:353320
TITLE: Preparation of amino(oxo)acetic acid derivatives as selective protein tyrosine phosphatase inhibitors
INVENTOR(S): Liu, Gang; Xin, Zhili; Pei, Zhonghua; Li, Xiaofeng; Szczepankiewicz, Bruce G.; Janowick, David A.; Oost, Thorsten K.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 60 pp., Cont.-in-part of U.S. Pat. Appl. 2002 72,516.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002169157	A1	20021114	US 2002-85157	20020227
US 2002035137	A1	20020321	US 2001-918928	20010731
US 2002072516	A1	20020613	US 2001-941471	20010829

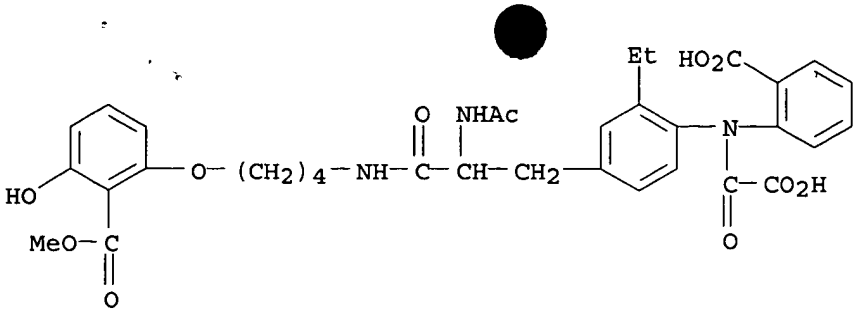
PRIORITY APPLN. INFO.: US 2000-228651P P 20000829
US 2000-650922 A2 20000829
US 2001-918928 A2 20010731
US 2001-941471 A2 20010829

OTHER SOURCE(S): MARPAT 137:353320

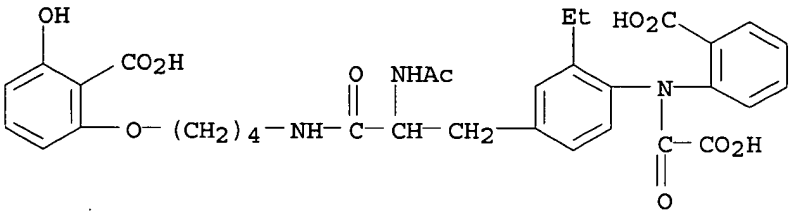
AB Compds. B-L-A-N(D)COCO2P2 [A are rings of defined structure; B = H, alkyl, aryl, arylalkyl, heterocyclyl, or heterocyclylalkyl; D = substituted Ph, alkyl, or 1-alkenyl [the substituent at the o- or 2-position is alkoxy, alkyl, sulfamoyl, amino, cyano, nitro, CO2P1, SO3H, P(O)(OH)2, CH2P(O)(OH)2, CHFP(O)(OH)2, CF2P(O)(OH)2, or C(:NH)NH2] or certain 5-membered heterocycles; P1, P2 = H, alkyl, alkenyl, arylalkyl, cycloalkyl, cycloalkylalkyl; L = (un)substituted (hetero)alkylene] or their therapeutically acceptable salts were prepd. as protein tyrosine kinase 1B (PTP1B) inhibitors. Thus, N-[5-[[N-acetyl-4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenylalanyl]amino]pentanoyl]-L-methionine and Me 2-[4-[[N-acetyl-4-[(carboxycarbonyl)(2-carboxyphenyl]amino]-3-ethylphenylalanyl)amino]butoxy]-6-hydroxybenzoate were prepd. and showed Kic = 0.077 .+-. 0.012 and 0.016 .+-. 0.003 .mu.M, resp., for inhibition of PTP1B.

IT **436864-07-2P 436864-18-5P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of amino(oxo)acetic acid derivs. as selective protein tyrosine phosphatase inhibitors)

RN 436864-07-2 CAPLUS
CN Benzoic acid, 2-[4-[[2-(acetylamino)-3-[4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenyl]-1-oxopropyl]amino]butoxy]-6-hydroxy-, 1-methyl ester (9CI) (CA INDEX NAME)



RN 436864-18-5 CAPLUS
CN Benzoic acid, 2-[4-[[2-(acetylamino)-3-[4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenyl]-1-oxopropyl]amino]butoxy]-6-hydroxy- (9CI) (CA INDEX NAME)



L7 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2002:450342 CAPLUS
DOCUMENT NUMBER: 137:33535
TITLE: Preparation of amino(oxo)acetic acids as selective protein tyrosine phosphatase inhibitors
INVENTOR(S): Liu, Gang; Szczepankiewicz, Bruce G.; Pei, Zhonghua; Xin, Zhili; Janowick, David A.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 44 pp., Cont.-in-part of U.S. Ser. No. 918,928.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002072516	A1	20020613	US 2001-941471	20010829
US 2002035137	A1	20020321	US 2001-918928	20010731
US 2002169157	A1	20021114	US 2002-85157	20020227
WO 2003020688	A1	20030313	WO 2002-US24506	20020801

W: CA, JP, MX
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR

PRIORITY APPLN. INFO.:
US 2000-228651P P 20000829
US 2000-650922 A2 20000829
US 2001-918928 A2 20010731
US 2001-941471 A2 20010829

OTHER SOURCE(S): MARPAT 137:33535
AB Compds. B-L-A-N(D)COCO2P2 [A are rings of defined structure; B = H, alkyl, aryl, arylalkyl, heterocyclyl, or heterocyclylalkyl; D = substituted Ph, alkyl, or 1-alkenyl, in which the substituent at the o- or 2-position is alkoxy, alkyl, amino, cyano, nitro, CO2P1, SO3H, P(O)(OH)2, CH2P(O)(OH)2, CHFP(O)(OH)2, CF2P(O)(OH)2, C(:NH)NH2, or certain 5-membered heterocycles; P1, P2 = H, alkyl, alkenyl, arylalkyl, cycloalkyl, cycloalkylalkyl; L = (un)substituted (hetero)alkylene] or their therapeutically acceptable salts were prepd. as protein tyrosine kinase 1B (PTP1B) inhibitors. Thus, N-[5-[[N-acetyl-4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenylalanyl]amino]pentanoyl]-L-methionine and Me

2-[4-[[N-acetyl-4-[(carbo[redacted]arbonyl)(2-carboxyphenyl]amino[redacted]-ethylphenylalanyl)amino]butoxy]-6-hydroxybenzoate were prepd. and showed Kic = 0.077 .+-. 0.012 and 0.016 .+-. 0.003 .mu.M, resp., for inhibition of PTP1B.

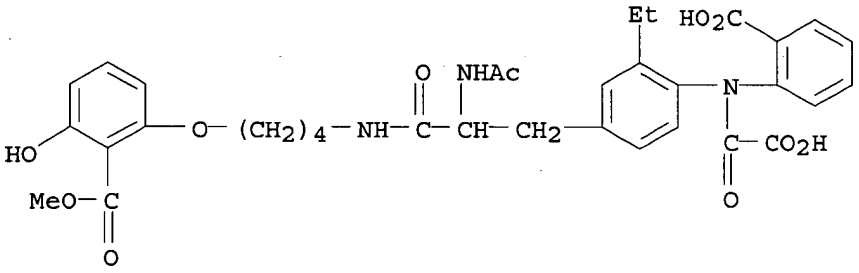
IT **436864-07-2P 436864-18-5P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of amino(oxo)acetic acids as selective protein tyrosine phosphatase inhibitors)

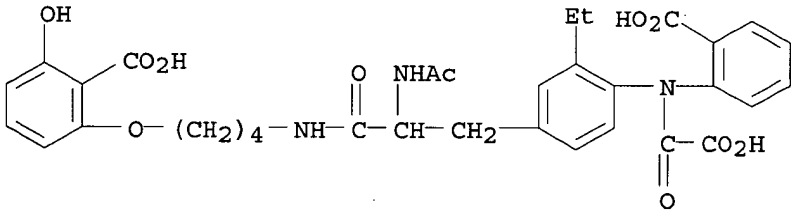
RN 436864-07-2 CAPLUS

CN Benzoic acid, 2-[4-[[2-(acetylamino)-3-[4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenyl]-1-oxopropyl]amino]butoxy]-6-hydroxy-, 1-methyl ester (9CI) (CA INDEX NAME)



RN 436864-18-5 CAPLUS

CN Benzoic acid, 2-[4-[[2-(acetylamino)-3-[4-[(carboxycarbonyl)(2-carboxyphenyl)amino]-3-ethylphenyl]-1-oxopropyl]amino]butoxy]-6-hydroxy- (9CI) (CA INDEX NAME)



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